Supporting Information

for

"A Polar Copper–Boron One-Electron Sigma Bond"

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Contents

Experimental Part

General Considerations. All manipulations were carried out using standard Schlenk or glovebox techniques under an N_2 atmosphere. Unless otherwise noted, solvents were deoxygenated and dried by thoroughly sparging with Ar gas followed by passage through an activated alumina column in the solvent purification system by SG Water, USA LLC. Non-halogenated solvents were tested with a standard purple solution of sodium benzophenone ketyl in tetrahydrofuran in order to confirm effective oxygen and moisture removal. All reagents were purchased from commercial vendors and used without further purification unless otherwise stated. TPB (**1**) was synthesized according to a literature procedure.[1] Elemental analyses were performed by Midwest Microlab, LLC., Indianapolis, IN. Deuterated solvents were purchased from Cambridge Isotope Laboratories, Inc., degassed, and dried over activated 3-Å molecular sieves prior to use. Deuterated THF was dried over NaK alloy prior to use. ^{1}H and ^{13}C chemical shifts are reported in ppm relative to tetramethylsilane, using residual solvent proton and ^{13}C resonances

[1] S. Bontemps, G. Bouhadir, P. W. Dyer, K. Miqueu, D. Bourissou, *Inorg. Chem.* **2007,** *46,* 5149-5151.

as internal standards. ^{31}P, ^{11}B, and ^{29}Si chemical shifts are reported in ppm relative to 85% aqueous H_3PO_4, $BF_3 \bullet Et_2O$, and tetramethylsilane, respectively. Multiplicities are indicated s (singlet), d (doublet), t (triplet), dd (double doublet), while apparent singlets, doublets, and triplets are indicated by "s", "d", and "t", respectively. Solution phase magnetic measurements were performed by the method of Evans.[2] X-band EPR spectra were obtained on a Bruker EMX spectrometer and simulated using Easyspin.[3] Optical spectroscopy measurements were taken on a Cary 50 UV-Vis spectrophotometer using a 1-cm two-window quartz cell.

X-Ray Crystallography. XRD studies were carried out at the Beckman Institute Crystallography Facility on a Bruker Kappa Apex II diffractometer (Mo Kα radiation). Structures were solved using SHELXS[4] and refined against F^2 on all data by full-matrix least squares with SHELXL. The crystals were mounted on a glass fiber. Relevant details are reported in Table 1.

Cu K-Edge XANES. Cu K-edge X-ray absorption near edge structure (XANES) for the single crystal samples were collected on the single crystal diffraction beamline 12-2 at Stanford Synchrotron Radiation Lightsource (SSRL) by utilizing the MAD capability of the beamline. The samples were mounted on a single axis goniometer with its rotation axis in the storage ring plane and perpendicular to the X-ray beam path; the XANES measurements were carried out by monitoring the Cu Kα fluorescence yield using a single-element Si drift detector (Vortex-90EX, SII NanoTechnology) lying in the storage ring plane perpendicular to the X-ray beam path (opposite to the goniometer). The single crystals were kept in a nitrogen stream at 100 K during data collection. In these measurements the storage ring was in its top-up injection mode and the intensity variation along the undulator peak within the XANES photon energy range was ignored. The XANES spectra of Cu powder were collected for photon energy calibration before and after the measurement on the single crystal samples and the first energy inflection of the

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[2] a) D. F. Evans, *J. Chem. Soc.* **1959,** 2003-2005; b) S. K. Sur, *J. Magn. Reson.* **1989,** *82,* 169-173.

[3] S. Stoll, A. Schweiger, *J. Magn. Reson.* **2006**, *178*(1), 42-55.

[4] Sheldrick, G. M. *Acta. Cryst.* **2008**, *A64*, 112.

copper metal spectra was assigned to 8980.3 eV. Two consistency tests were carried out to ensure that no X-ray beam damage to the single crystal samples: 1) no XANES feature variation was observed among the multiple scans of the data collection; 2) The crystallographic diffraction data of the single crystals were collected after XANES data collection and the refined crystallographic structure were compared with those collected previously (see X-ray Crystallography section) to assure no change to the crystallographic structure. The angles between the polarization vector $\vec{e}$ and the Cu–B bond are 164°, 153° and 95° for {(TPB)Cu}{BAr^F_4}, (TPB)Cu, and {K(benzo-15-C-5)$_2$}{(TPB)Cu}, respectively. The XANES data reductions (merge of data from all orientations, pre-edge background removal and energy calibration) were processed by using Arthena[5]. The acquired XANES spectra were first stripped off the pre-edge background by fitting a linear function and then normalized at energy 9010 eV.

[5] B. Ravel, M. Newville, *J. Synchrotron Rad.* **2005**, 12, 537 - 541

Computational Methods. Geometry optimizations were performed using the Gaussian03 package[6] using the XRD geometries as starting point. The B3LYP exchange-correlation functional was employed with a 6-31+G(d) basis set. The GDIIS algorithm was used. A full frequency calculation was performed on each structure to ensure that they are true minima. NBO[7] analyses were performed on the electron density obtained at the B3LYP/6-311+G(d,p)//6-31+G(d) level.

(TPB)Cu. A mixture of TPB (245 mg, 42 mmol) and CuBr (64 mg, 45 mmol) in THF (6 mL) was stirred for 15 minutes, resulting in a yellow solution. Freshly prepared sodium amalgam (15 mg, 65 mmol Na; 3.5 g Hg) was added, and the mixture was vigorously stirred for 17 h. The volatiles were removed *in*

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[6] Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

[7] (a) Feed, A. E.; Curtiss, L. A.; Weinhold, F. *Chem. Rev.* **1988**, 899. (b) Weinhold, F.; Landis, C. R. Valency and Bonding: A Natural Bond Orbital Donor-Acceptor Perspective; Cambridge University Press: New York, 2005.

vacuo, and the dark residue was extracted with benzene (4 + 3 × 1 mL) to yield an inky purple solution. Slow evaporation of the solvent afforded the product as black blocks that were washed with pentane (3 × 0.5 mL) and dried *in vacuo*. Yield: 140 mg, 50 %. ^{1}H NMR (C_6D_6, 300 MHz): δ 13 (v br), 3(v br), 1 (v br), –5 (v br). UV-Vis (THF, nm {$cm^{-1}M^{-1}$}): 665 {2300}, 485 {4200}, 345 {6400}, 310 {sh}. Anal: calcd for $C_{36}H_{54}BCuP_3$: C 66.07, H 8.32; found: C 65.93, H 8.29. Crystals suitable for XRD were grown by slowly concentrating a solution of (TPB)Cu in pentane by vapor diffusion into hexamethyldisiloxane.

[(TPB)Cu][BAr$^{F}_{4}$]. A mixture of TPB (20 mg, 34 μmol), CuBr (5mg, 35 μmol) and Na[BAr$^{F}_{4}$] (31 mg, 35 μmol) in diethyl ether (2 mL) was stirred for 2.5 hours to yield a yellow suspension. The white precipitate was removed by filtration, and the yellow solution was slowly concentrated by vapor diffusion into methylcyclohexane. Decantation, washing with pentane (0.5 mL) and benzene (0.5 mL), and drying *in vacuo* afforded the product as yellow blocks (36 mg, 70%). ^{1}H NMR (CD_2Cl_2, 400 MHz): δ 7.73 (8H, br, BAr$^{F}_{4}$ *ortho*-H), 7.62 (3H, br, Ar–H^{6}), 7.57 (4H, br, BAr$^{F}_{4}$ *para*-H), 7.42 (m, 6H, Ar–H^{4,5}), 6.95 (3H, d, ^{3}J(H–H) = 7.2 Hz, Ar–H^{3}), 2.58 (3H, m, PC*H*), 2.25 (3H, m, PC*H*), 1.51 (18H, m, CH_3), 0.81 (9H, m, CH_3), 0.55 (9H, m, CH_3). ^{13}C NMR (CD_2Cl_2, 100 MHz): δ 162.4 (q, ^{1}J(^{11}B–C) = 50 Hz, BAr$^{F}_{4}$ B*C*), 158 (br, *C*^{Ar}) 135.4 (s, BAr$^{F}_{4}$ *ortho-C*), 133.1 ('q', *J* = 11.4 Hz, *C*^{Ar}), 131.9 ('q', *J* = 6.1 Hz, *C*^{Ar}), 131.5 (s, *C*^{Ar}), 130.9 (s, *C*^{Ar}), 130.1 (s, *C*^{Ar}), 129.5 (q, ^{2}J(F–C) = 31.9 Hz, BAr$^{F}_{4}$ *meta-C*), 125.2 (q, ^{1}J(F–C) = 272.5 Hz, *C*F$_3$), 118.1 (m, BAr$^{F}_{4}$ *para-C*), 27.3 ('q', *J* = 6 Hz, P*C*H), 26.6 (m, P*C*H), 24.9 ('q', *J* = 4 Hz, C*C*H$_3$), 19.6 (s, C*C*H$_3$), 19.2 (s, C*C*H$_3$), 18.6 (s, C*C*H$_3$). ^{31}P NMR (CD_2Cl_2, 121 MHz): δ 19.3. ^{11}B NMR (CD_2Cl_2, 128 MHz): δ 67 (br, [(TPB)Cu]), –6.6 (BAr$^{F}_{4}$). UV-Vis (THF, nm {$cm^{-1}M^{-1}$}): 430 {sh}, 403 {850}, 320 {8000}. Anal: calcd for $C_{68}H_{66}B_2CuF_{24}P_3$: C 53.79, H 4.38; found: C 53.96, H 4.39. Crystals suitable for XRD were grown by slowly concentrating a solution of [(TPB)Cu][BAr$^{F}_{4}$] in diethyl ether by vapor diffusion into hexamethyldisiloxane.

[(TPB)Cu]Na. An inky purple solution of (TPB)Cu in 1:10 THF-d_8 / benzene-d_6 (0.5 mL) was stirred over an excess of metallic sodium for 1 h and the resulting inky blue solution was transferred to a quartz

J-Young NMR tube. ^{1}H NMR (300 MHz): δ 7.2 (br sh, 3H, Ar–*H*) 6.5 (br, 9H Ar–*H*), 2.1 (br, 6H, PC*H*), 1.3 (br, 36H, CH_3). ^{31}P NMR (121 MHz): δ 20.1. ^{11}B NMR (128 MHz): δ 6.7.

[(TPB)Cu][K(Bz-15-c-5)$_2$]. An inky purple suspension of (TPB)Cu (30 mg, 46 μmol) in diethyl ether (1 mL) was stirred over metallic potassium (13 mg, 0.33 mmol) for 1 h. The resulting inky blue solution was transferred to a J-Young Schlenk tube and layered with a solution of benzo-15-crown-5 (31 mg, 116 μmol) in diethylether (2 mL) and left standing for 12 h. Decantation, washing with diethyl ether, and drying *in vacuo* afforded the product as black plates suitable for XRD (47 mg, 83%) . UV-Vis (DEE, nm {cm^{-1}M^{-1}}): 780 {sh}, 615 {4900}, 530 {5100}, 350 {sh}. Anal: calcd for $C_{64}H_{94}BCuKO_{10}P_3$: C 62.48, H 7.71; found: C 62.10, H 7.13.

NMR Spectra

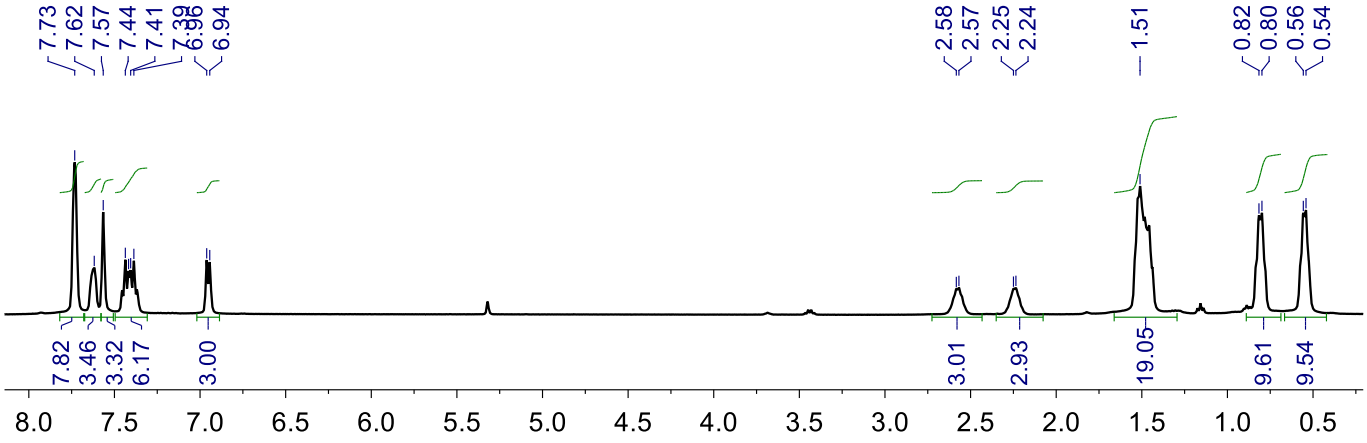

Figure S1. ^{1}H NMR spectrum of [(TPB)Cu]BAr$^{F}_{4}$ in CD_2Cl_2 at room temperature.

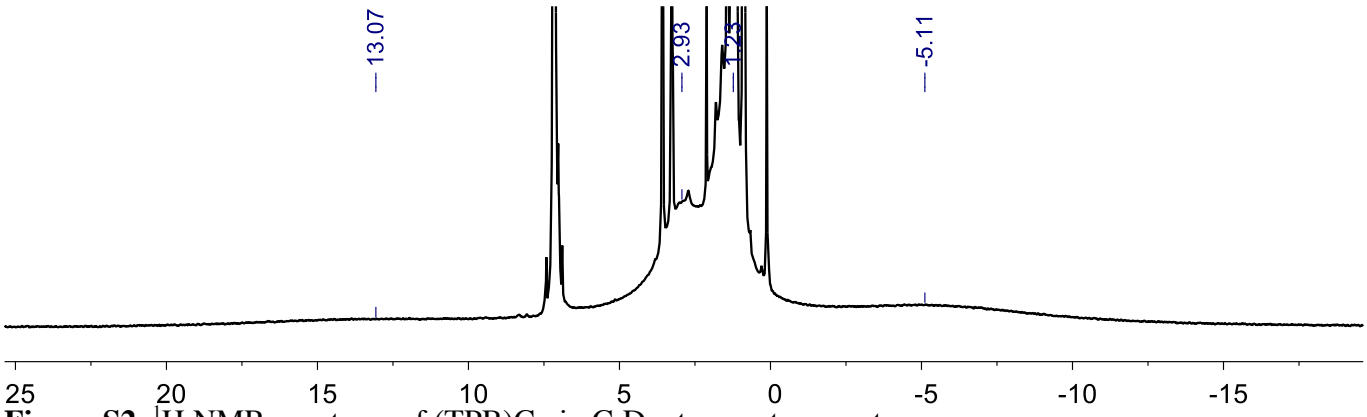

Figure S2. ^{1}H NMR spectrum of (TPB)Cu in C_6D_6 at room temperature.

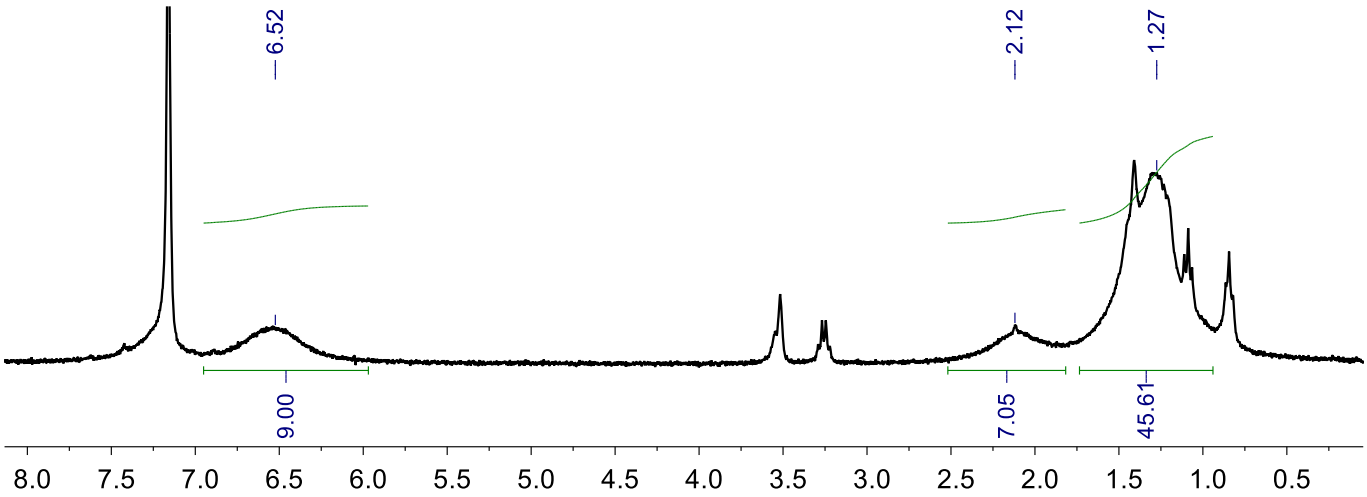

Figure S3. ^{1}H NMR spectrum of Na[(TPB)Cu] generated *in situ* in 1:10 THF-d_8/C_6D_6 at room temperature.

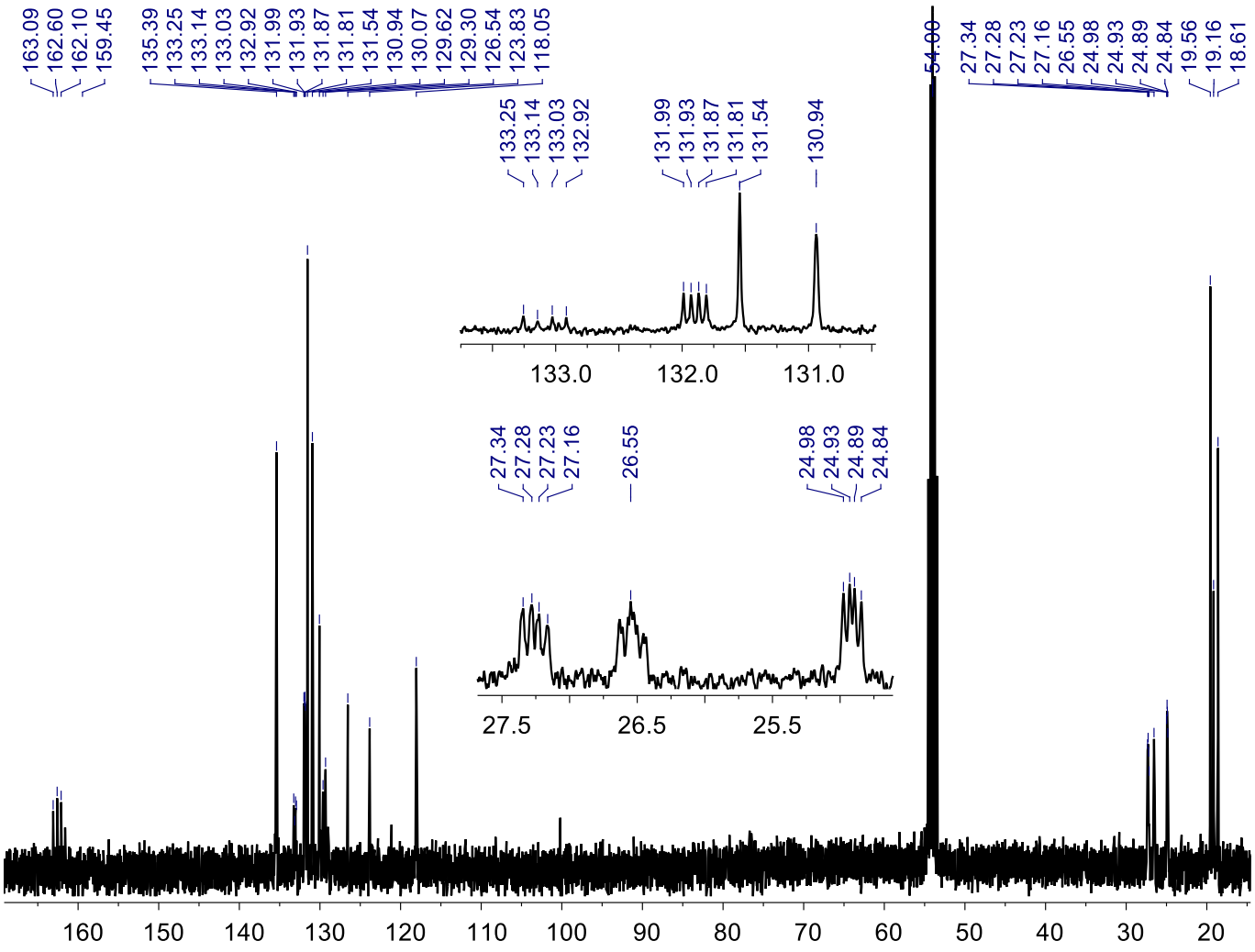

Figure S4. ^{13}C NMR spectrum of [(TPB)Cu]BAr^F_4 in CD_2Cl_2 at room temperature.

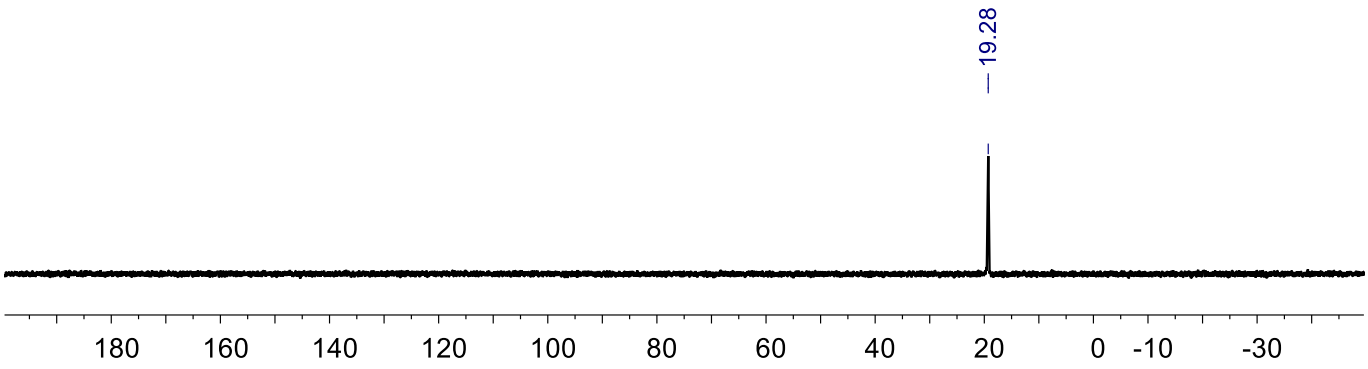

Figure S5. ^{31}P NMR spectrum of [(TPB)Cu]BAr^F_4 in CD_2Cl_2 at room temperature.

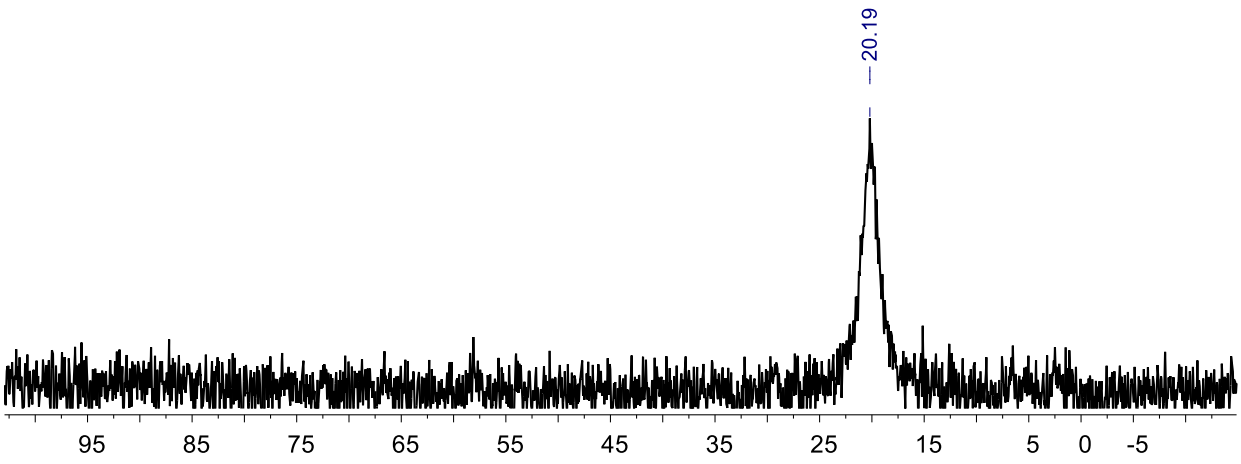

Figure S6. ^{31}P NMR spectrum of Na[(TPB)Cu] generated *in situ* in 1:10 THF-d_8/C_6D_6 at room temperature.

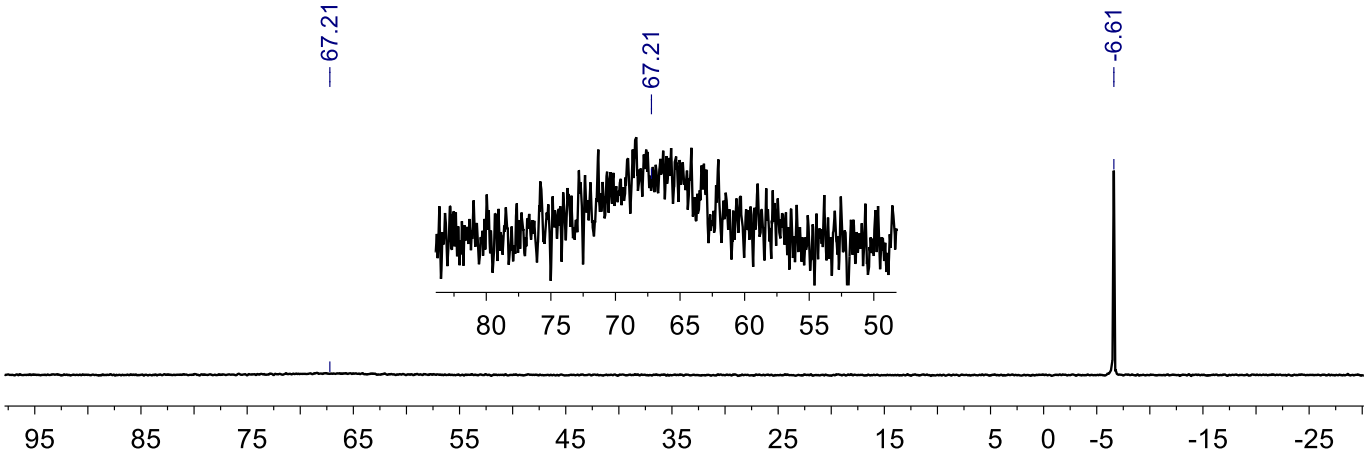

Figure S7. ^{11}B NMR spectrum of [(TPB)Cu]BAr^F_4 in CD_2Cl_2 at room temperature.

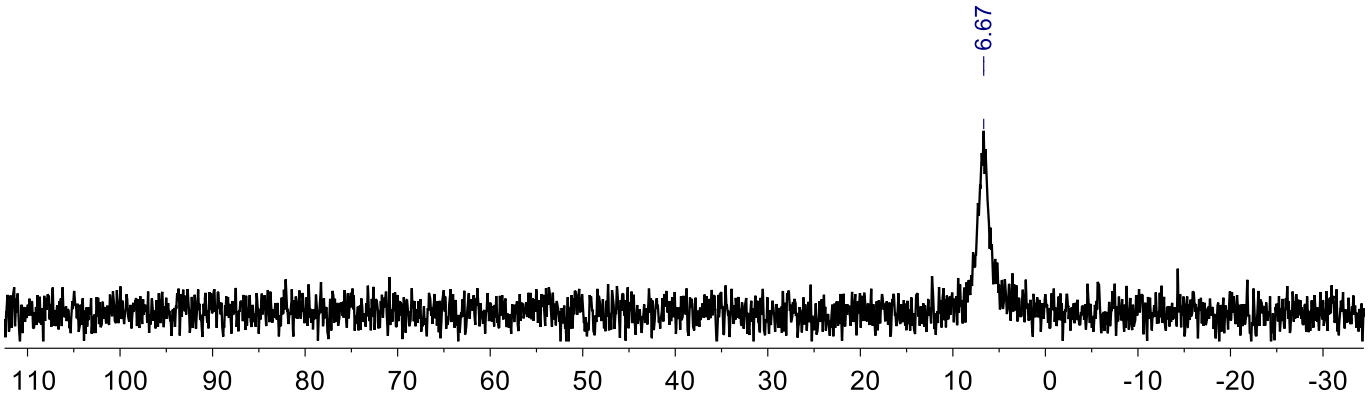

Figure S8. ^{11}B NMR spectrum of Na[(TPB)Cu] generated *in situ* in 1:10 THF-d_8/C_6D_6 at room temperature.

EPR Spectra

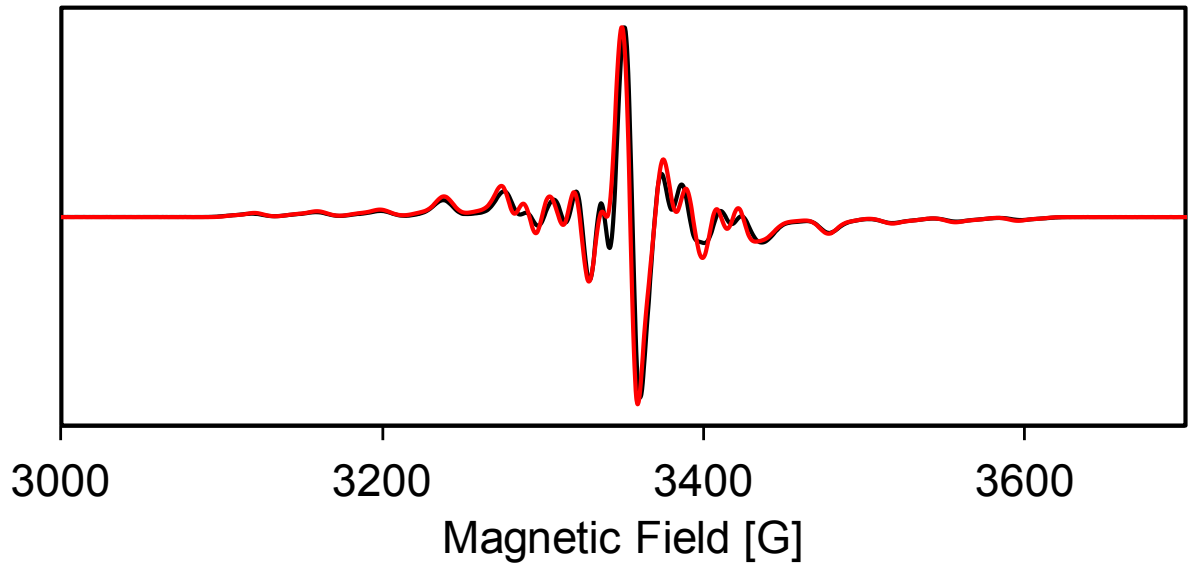

Figure S9. X-band EPR spectrum of (TPB)Cu in toluene at 77 K (black) and simulated spectrum (red). Simulation parameters: $g_{\parallel} = 2.006$, $g_{\perp} = 2.0099$, $A_{\parallel}[B] = 110$ MHz, $A_{\perp}[B] = 40$ MHz, $A_{\parallel}[Cu] = 335$ MHz, $A_{\perp}[Cu] = 93$ MHz.

UV-Vis Spectra

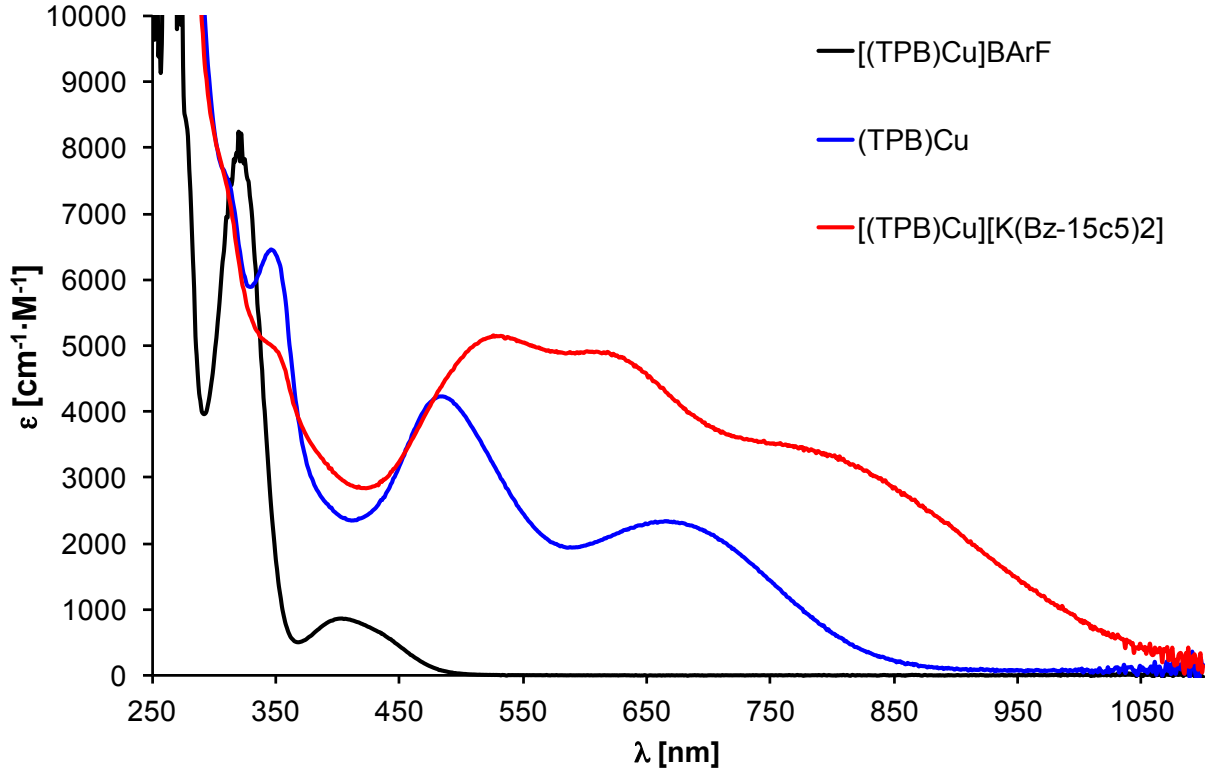

Figure S10. UV-Vis spectra of (TPB)Cu (0.16 mM in THF, blue), [(TPB)Cu]BAr^F_4 (0.37 mM in THF, black), and [(TPB)Cu][$K(Bz\text{-}15\text{-}c\text{-}5)_2$] (0.15 mM in diethylether, red).

X-Ray Diffraction Data

Table 1: Crystallographic Data for Compounds {(TPB)Cu}{BAr^F_4}, (TPB)Cu, and {K(benzo-15-C-5)$_2$}{(TPB)Cu}

	(TPB)Cu	**{(TPB)Cu}{BAr^F_4}**	**{K(benzo-15-C-5)$_2$}{(TPB)Cu}**
chem formula	$C_{36}H_{54}BCuP_3$	$C_{68}H_{66}B_2CuF_{24}P_3$	$C_{64}H_{94}BCuKO_{10}P_3$
fw	654.05	1517.28	1229.75
cryst syst	Triclinic	Orthorhombic	Monoclinic
space group	P-1	Pbca	$P2_1/c$
a [Å]	10.9624(4)	26.2296(12)	11.3982(5)
b [Å]	11.1511(4)	19.7982(9)	34.9481(15)
c [Å]	16.6631(7)	26.5304(11)	16.0773(7)
α [°]	77.562(2)	90	90
β [°]	78.236(2)	90	92.586(2)
γ [°]	61.599(2)	90	90
V [Å^3]	1737.48(12)	13777.2(11)	6397.8(5)
Z	2	8	4
D_{calcd} [g cm^{-3}]	1.250	1.463	1.277
F(000)	698.0	6192.0	2624.0
μ [mm^{-1}]	0.790	0.493	0.537
temp. [K]	100	100	100
wavelength [Å]	0.71073	0.71073	0.71073
measd rflns	92896	376881	242329
unique rflns	25085	34263	32108
data/restraints/param	25085/0/382	34263/109/981	32108/0/733
R(F) (I>2σ(I))	0.0497	0.0461	0.0411
wR(F^2) (all)	0.1144	0.1299	0.0952
GOF	1.036	1.042	1.020

DFT Calculations

Optimized Coordinates [Å] for (TPB)Cu

Atom	X	Y	Z
Cu	-0.00037400	-0.00073200	-0.90014900
P	0.57234800	2.28283800	-0.76953600
P	-2.26283400	-0.64678600	-0.77050600
P	1.69270900	-1.63538600	-0.76952200
C	-0.16647800	2.64425700	0.88649600
C	2.37323800	-1.17894300	0.88801500
C	-1.08141800	-1.78442700	2.99157600
H	-0.26168100	-1.56468600	3.67281900
C	-2.20960600	-1.46288300	0.88791500
C	1.44883400	-3.52994900	-0.66876000
H	0.87848800	-3.77294000	-1.57398500
C	2.33468100	3.01878600	-0.66527800
H	2.83118800	2.64872100	-1.57099400
C	-3.78099300	0.51258500	-0.67387300
H	-3.70244600	1.12896700	-1.57810500
C	-0.39316800	1.53496600	1.75134500
C	-3.15543300	-2.43002100	1.27106200
H	-3.95662700	-2.71095900	0.59204400
C	3.12848100	-1.52504300	-1.99921900
H	3.93601300	-2.17352900	-1.63937900
C	3.68440700	-1.51214600	1.27088600
H	4.32945300	-2.06404800	0.59174400
C	-1.00810400	1.82768800	2.99036100
H	-1.22551600	1.00804600	3.67245200
C	-0.53585300	3.94616800	1.26764800
H	-0.38048900	4.78015300	0.58780100
C	1.52550800	-0.42795300	1.75252800
C	-1.36804800	3.12137400	3.37052700
H	-1.84057600	3.29238400	4.33595400
C	-1.13417300	-1.10659600	1.75193600
C	-2.88423700	-1.94778100	-1.99857700
H	-3.85174500	-2.31930100	-1.64072300
C	-3.07200600	-3.06940400	2.50888500
H	-3.80622100	-3.82189400	2.78702200
C	-0.23905900	3.47176000	-2.00007100
H	-0.08386500	4.49509400	-1.63831000
C	-3.70246900	1.44201800	0.54587700
H	-4.52263700	2.17112200	0.50405900
H	-2.76263200	1.99191600	0.59926600
H	-3.80510800	0.87558000	1.47765200
C	2.08517500	-0.04351900	2.99265000
H	1.48381000	0.55468700	3.67446000
C	-1.13350800	4.19304100	2.50452500
H	-1.42192900	5.20446800	2.78111700
C	-2.02477400	-2.73930200	3.37364700
H	-1.93757800	-3.23312000	4.33962700
C	-1.74861400	3.24100900	-2.13163300
H	-2.17357200	3.95914500	-2.84584200
H	-2.26920900	3.36746600	-1.17845000
H	-1.95702000	2.23294100	-2.50675700
C	0.60170100	-3.92474100	0.54950000
H	0.38376300	-5.00039500	0.51074300
H	-0.34633200	-3.38857900	0.59742200
H	1.13955200	-3.72543800	1.48253100
C	-5.15493000	-0.18073100	-0.68899500
H	-5.28581700	-0.83183100	0.18239900
H	-5.33804000	-0.77050300	-1.59205200
H	-5.94015600	0.58567400	-0.63973000
C	-1.93431200	-3.14451100	-2.11912100
H	-2.34218200	-3.87224600	-2.83358100
H	-1.79269600	-3.65577000	-1.16306100
H	-0.95294400	-2.82714500	-2.48843300
C	0.43728600	3.32929700	-3.37598700
H	0.31860500	2.31001500	-3.76473300
H	1.50847700	3.55544700	-3.35053800
H	-0.02779000	4.01614400	-4.09534000
C	-3.08808200	-1.29585300	-3.37854200
H	-2.14161300	-0.89611400	-3.76390900
H	-3.81485100	-0.47685500	-3.36055500
H	-3.45091600	-2.04310100	-4.09652800
C	3.38448800	-0.38072300	3.37445300
H	3.76784200	-0.05845900	4.34076500
C	2.73717300	-4.37185100	-0.67853200
H	3.36308700	-4.15824800	0.19494700
H	3.34272600	-4.23557900	-1.57945100
H	2.46701300	-5.43532800	-0.62940400
C	3.68582700	-0.10291500	-2.12657000
H	4.51824200	-0.09275000	-2.84307900
H	4.05917200	0.28017800	-1.17291700
H	2.91732200	0.58461800	-2.49673300
C	2.41888300	4.55552000	-0.67082100
H	1.92097400	4.98785100	0.20413500
H	1.99756000	5.01420500	-1.57025700
H	3.47482300	4.85368400	-0.62113300
C	3.09937300	2.47989000	0.55227800
H	4.13947700	2.83043900	0.51577000
H	3.11037500	1.39067600	0.59684200
H	2.65632400	2.84265200	1.48591900
C	4.19559700	-1.11999900	2.50899300
H	5.21493900	-1.37764600	2.78689900
C	2.66607400	-2.03476300	-3.37663100
H	1.84512100	-1.41855000	-3.76446600
H	2.32256900	-3.07434000	-3.35368700
H	3.49412800	-1.97672700	-4.09529200
B	-0.00002200	-0.00015700	1.40996900

Optimized Coordinates [Å] for [(TPB)Cu][BAr^F_4]

Atom	X	Y	Z
Cu	0.03066900	-0.05472000	-0.96808200
P	2.29377500	-0.73523000	-0.72486100
C	2.82090300	-2.05443500	-1.96332400
C	1.79774300	-3.18593400	-2.08819600
H	0.84803900	-2.80707200	-2.47812200
H	1.60581200	-3.68019400	-1.13174200

H	2.16787700	-3.94442200	-2.78895800
C	3.07273000	-1.40512700	-3.33745800
H	3.39425800	-2.17162700	-4.05268900
H	3.85044800	-0.63561700	-3.31256800
H	2.15694900	-0.94961500	-3.73465200
P	-1.84252700	-1.49144800	-0.62223000
P	-0.50843000	2.25158500	-0.78864400
C	0.93893900	-1.87788400	2.99440800
H	0.11532200	-1.63641100	3.66127700
C	1.07919800	-1.16835900	1.78124200
C	-2.10993800	-3.36450000	-0.63284000
H	-3.16013000	-3.48829700	-0.33616300
C	-2.25416300	3.01498000	-0.73722500
H	-2.74094200	2.59493400	-1.62850600
C	1.31413700	4.20488300	2.38751600
H	1.60924200	5.22180800	2.63115900
C	3.01263100	-2.59170600	1.29890800
H	3.80655100	-2.90832700	0.62898300
C	2.14665200	-1.55363900	0.92322800
C	0.54664800	1.55403100	1.72577500
C	0.27259900	2.63175100	0.84097900
C	3.82189900	1.31525200	0.56628100
H	3.85965900	0.77525500	1.51825100
H	2.93052000	1.94282600	0.57214900
H	4.69804500	1.97364700	0.52337700
C	1.22574300	1.85228300	2.92584100
H	1.48210200	1.04540600	3.60889200
C	-3.17145500	-0.77459300	-1.77700100
H	-3.32047800	0.23216500	-1.36772800
C	-2.30308200	4.54995700	-0.84340800
H	-3.35204700	4.87053500	-0.83273800
H	-1.85894200	4.94051400	-1.76270400
H	-1.81321800	5.02887100	0.01150600
C	0.67116200	3.93487200	1.17710900
H	0.49437900	4.75469900	0.48691000
C	1.58957400	3.15721100	3.26624700
H	2.10413900	3.34871700	4.20421800
C	-3.04671700	2.56579600	0.49990300
H	-2.59641900	2.95276700	1.42010200
H	-3.11470500	1.48112200	0.59365100
H	-4.06739000	2.96223000	0.43752000
C	-1.48062800	-0.25892900	1.88676800
C	-1.94971600	0.19291700	3.13936900
H	-1.31536700	0.83244100	3.74843900
C	-4.04115300	-0.97922100	2.86554400
H	-5.01902000	-1.27277400	3.23734500
C	-3.20549100	-0.16622300	3.63172900
H	-3.52835400	0.19030000	4.60637500
C	-3.61907900	-1.40141700	1.60366400
H	-4.28866700	-2.02101700	1.01662200
C	2.86855200	-3.24963800	2.52270300
H	3.55500300	-4.04642300	2.79586700
C	1.82674100	-2.88704300	3.37483100
H	1.68920900	-3.39878400	4.32374200
C	3.86018200	0.34627600	-0.62341200
H	3.82590500	0.93780500	-1.54669100
C	-1.93329300	-4.02369400	-2.01011100
H	-0.90883000	-3.93235000	-2.38053200
H	-2.60624000	-3.61348000	-2.76781800
H	-2.15490600	-5.09464700	-1.92564500
C	-4.54142700	-1.47155100	-1.81591400
H	-5.20024800	-0.92832000	-2.50491200

Optimized Coordinates [Å] for [(TPB)Cu][K(Bz-15-c-5)$_2$].

Atom	X	Y	Z
Cu	0.00000000	0.00000000	0.89818000
P	1.71703800	1.59149300	0.70552100
P	0.51975400	-2.28274500	0.70552100
P	-2.23679200	0.69125200	0.70552100
C	-0.61302300	-1.43478400	-1.69092900
C	1.54907100	0.18649900	-1.69092900
C	-1.43031200	-1.65167500	-2.83096300
H	-1.74086100	-0.78499100	-3.41296300
C	-0.27996900	-2.60504100	-0.93437000
C	2.39601600	1.06006000	-0.93437000
C	-2.11604700	1.54498100	-0.93437000
C	-0.93604800	1.24828600	-1.69092900
C	-0.71523600	2.06452400	-2.83096300
H	0.19060900	1.90012600	-3.41296300
C	0.00000000	-3.77935500	1.80761800
H	0.55997600	-4.66956800	1.48195300
C	1.11337700	3.37937500	0.38285600
H	0.13674200	3.20299700	-0.08108500
C	2.14554800	-0.41284900	-2.83096300
H	1.55025300	-1.11513500	-3.41296300
C	2.36993600	-2.65390000	0.38285600
H	2.70550600	-1.71992000	-0.08108500
C	3.66982200	1.42153200	-1.40772800
H	4.27410800	2.14246000	-0.85985300
B	0.00000000	0.00000000	-1.32333900
C	-3.06599400	2.46739300	-1.40772800
H	-3.99247900	2.63025600	-0.85985300
C	-0.60382800	-3.88892600	-1.40772800
H	-0.28162900	-4.77271600	-0.85985300
C	-1.62682100	3.02829400	-3.25898500
H	-1.41882200	3.61468500	-4.15409900
C	-2.83345600	3.21280200	-2.56388700
H	-3.56971400	3.93754000	-2.90751200
C	-3.27301800	1.88967800	1.80761800
H	-4.32395300	1.84983000	1.48195300
C	4.19909600	0.84744300	-2.56388700
H	5.19486600	1.12269300	-2.90751200
C	3.43599000	-0.10527900	-3.25898500
H	3.83982000	-0.57860700	-4.15409900
C	-1.80916900	-2.92301500	-3.25898500
H	-2.42099800	-3.03607900	-4.15409900
C	-3.48331300	-0.72547500	0.38285600
H	-2.84224800	-1.48307700	-0.08108500
C	3.27301800	1.88967800	1.80761800
H	3.76397600	2.81973800	1.48195300
C	-1.36564000	-4.06024500	-2.56388700
H	-1.62515200	-5.06023300	-2.90751200
C	-1.50548800	-4.08150800	1.73052800
H	-1.74968500	-4.92920600	2.38787900
H	-1.84967700	-4.32177700	0.72309300
H	-2.08386600	-3.22016300	2.08007800
C	2.84746700	2.03799600	3.28513300
H	2.31519300	1.13719200	3.61814200

H	2.19058200	2.89034800	3.46820400
H	3.73641000	2.15969600	3.92175200
C	3.20592100	-2.87815300	1.65102600
H	3.02833000	-3.87253300	2.08012000
H	3.00106800	-2.13251100	2.42523800
H	4.27553000	-2.81830900	1.40419300
C	-4.09551400	-1.33733300	1.65102600
H	-4.86787700	-0.68634400	2.08012000
H	-3.34734300	-1.53274500	2.42523800
H	-4.57849200	-2.29356300	1.40419300
C	2.63919200	-3.79930400	-0.61157500
H	3.72246100	-3.89759300	-0.77526900
H	2.16812500	-3.61877800	-1.58046200
H	2.27739600	-4.76474100	-0.23140800
C	-2.78194600	3.34454500	1.73052800
H	-3.39397500	3.97987500	2.38787900
H	-2.81793000	3.76275500	0.72309300
H	-1.74681000	3.41476300	2.08007800
C	-4.60989000	-0.38595500	-0.61157500
H	-5.23664500	-1.27494900	-0.77526900
H	-4.21801600	-0.06826200	-1.58046200
H	-5.26508500	0.41008700	-0.23140800
C	4.28743300	0.73696300	1.73052800
H	5.14366000	0.94933100	2.38787900
H	4.66760700	0.55902100	0.72309300
H	3.83067600	-0.19459900	2.08007800
C	1.97069800	4.18526000	-0.61157500
H	1.51418400	5.17254300	-0.77526900
H	2.04989100	3.68704000	-1.58046200
H	2.98768800	4.35465300	-0.23140800
C	0.88959300	4.21548600	1.65102600
H	1.83954700	4.55887700	2.08012000
H	0.34627500	3.66525600	2.42523800
H	0.30296300	5.11187200	1.40419300
C	0.34122300	-3.48497700	3.28513300
H	-0.17275900	-2.57361200	3.61814200
H	1.40782400	-3.34227400	3.46820400
H	0.00214700	-4.31567400	3.92175200
C	-3.18869000	1.44698100	3.28513300
H	-2.14243400	1.43642000	3.61814200
H	-3.59840600	0.45192500	3.46820400
H	-3.73855600	2.15597800	3.92175200